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14. ABSTRACT

The objective of this project was to develop an emerging, stabilized finite element method for treating general interfacial laws and microstructural representations independently of a background finite element mesh. Major research objectives and accomplishments associated with the project include: 1) extension of the basic approach to account for dissipative bulk and interfacial phenomena, such as crystal plasticity and grain boundary sliding, and the adaptation of the approach to explicit dynamics; 2) the leveraging of numerical analysis to greatly improve the efficiency of the method, and the exploitation of methods for multi-scale coupling to continuum models; and 3) the training of a broad range of graduate students in the use of these methods.

15. SUBJECT TERMS

embedded finite element methods, microstructural, multiscale

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Numerical Methods for Material Systems with Microstructure
Final Report
Submitted to AFOSR
December 14, 2012

Chandrasekhar Annavarapu[1] and John Dolbow[2]

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1 Objectives

The proposed work was based in large part on the PI's recent developments in stabilized finite element methods that enable the simulation of interfaces that are not explicitly gridded. The important point is that this approach provides a means to efficiently and robustly simulate the response of multiple instantiations of complex microstructures. The efficiency stems from the ability to use a single background mesh to simulate a full distribution of microstructural topologies. No remeshing is required, translating to significant cost savings and eliminating the need for analyst intervention. Further, we have carefully developed the method so that stabilization terms are determined as part of the formulation; there do not exist any "free parameters" that require analyst tuning. Accordingly, this proposal was designed to both improve on our basic approach as well as extend it to other important areas of interest in structural mechanics.

The objective of this project was to develop an emerging, stabilized finite element method for treating general interfacial laws and microstructural representations independently of a background finite element mesh. Major research objectives and accomplishments associated with the project, and the publicly available sources where these results were documented, are as follows:

- Extension of the basic approach to account for dissipative bulk and interfacial phenomena, such as crystal plasticity and grain boundary sliding, and the adaptation of the approach to explicit dynamics;
- The leveraging of numerical analysis to greatly improve the efficiency of the method, and the exploration of methods for multi-scale coupling to continuum models;
- The training of a broad range of graduate students in the use of these methods.

These methodologies were formulated within highly-portable subroutines and algorithms that could be easily incorporated by analysts into legacy finite element and emerging research codes.

2 Accomplishments / New Findings

The primary accomplishment of the work to date has been the development of stabilized methods useful for both fluid/structure and solid/solid interfaces, without the need for explicit gridding of such interfaces. Methods have been demonstrated both for simple fluid-structure interaction problems, as well as for application in which the "interfaces" are grain boundaries that are not explicitly meshed by the analyst.

In particular, we have developed a new form of Nitsche's method for embedded interface problems. The new formulation sets the weights in Nitsche's method and the stabilization parameter such that the method is robust for problems in which the interface separates materials with a high contrast in mechanical properties. It is also robust in the presence of extremely small partial elements. We have extended this method to problems in which the interfacial constitutive law is nonlinear (as in frictional contact) and when triple-junctions are present. The method is summarized in the publications associated with this project (see Section 4).

3 Personnel Supported

Personnel involved with this project over the past three years include:

- John E. Dolbow (PI), Professor, Department of Civil and Environmental Engineering, Duke University
- Jessica Sanders, Graduate Research Assistant, Department of Civil and Environmental Engineering, Duke University
- Chandrasekhar Annavarapu, Graduate Research Assistant, Department of Civil and Environmental Engineering, Duke University

4 Publications

During the period of time encompassed by this award, the PIs on this grant have submitted and published several works with direct relevance to this project:

- Dolbow, J. & I. Harari (2009), "An Efficient Finite Element Method for Embedded Interface Problems," *International Journal for Numerical Methods in Engineering*, **78**, 229–252.

- Harari, I. & J. Dolbow (2010), "Analysis of an Efficient Finite Element Method for Embedded Interface Problems," *Computational Mechanics*, **46**, 205–211.

- Sanders, J., J.E. Dolbow, P.J. Mucha, & T.A. Laursen (2011), "A New Method for Simulating Rigid Body Motion in Incompressible Two-Phase Flow," *International Journal for Numerical Methods in Fluids*, **67**, 713–732.

- Hautefeuille, M., C. Annavarapu, & J.E. Dolbow (2012), "Robust Imposition of Dirichlet Boundary Conditions on Embedded Surfaces," *International Journal for Numerical Methods in Engineering*, **90**, 40–64.

- Annavarapu, C., M. Hautefeuille, & J. Dolbow (2012), "A Robust Nitsche Formulation for Interface Problems," *Computer Methods in Applied Mechanics and Engineering*, **225-228**, 44–54.

- Annavarapu, C., M. Hautefeuille, & J.E. Dolbow (2012),"Stable Imposition of Stiff Constraints in Explicit Dynamics for Embedded Finite Element Methods," *International Journal for Numerical Methods in Engineering*, **92**, 206–228.

- Annavarapu, C., M. Hautefeuille, & J.E. Dolbow (2012), "A Nitsche Stabilized Formulation for Frictional Sliding Problems with Embedded Finite Element Methods," in preparation.

- Annavarapu, C., M. Hautefeuille, & J.E. Dolbow (2012), "A Nitsche Stabilized Formulation for Frictional Sliding Problems with Embedded Finite Element Methods - Part II: Intersecting Interfaces," in preparation.

5 Interactions / Transitions

5.1 Participation/ presentations at meetings and conferences

Presentations made at international meetings and workshops during the award period, with particular pertinence to this project include:

- Dolbow, J.E. "Numerical Methods for Material Systems with Microstructure," poster presented at AFOSR Multi-Scale Structural Mechanics Portfolio Review, Eglin AFB, August 17–19, 2010.

- Dolbow, J.E. "Embedded Finite Element Methods for Evolving Interface Problems," ENS de Cachan, invited seminar, Paris, France, October 15, 2010.

- Dolbow, J.E. "Recent Advances in Embedded Finite Element Methods," Workshop on Fluid Motion Driven by Immersed Structures, University of Toronto, Toronto, Canada, August 11, 2010.
- Hautefeuille, M. "Stable Imposition of Dirichlet Boundary Conditions and Stiff Constraints over Embedded Surfaces," 11th US National Congress on Computational Mechanics, July 25–28, 2011.
- Chandasekhar, A. "Robust Implementation of Stiff Constraints on Fixed Embedded Surfaces for Quasi-Static and Transient Problems," 11th US National Congress on Computational Mechanics, July 25–28, 2011.
- Chandasekhar, A. "A Robust Nitsche Formulation for Interface Problems," 10th World Congress on Computational Mechanics, Sao Paulo, Brazil, July 9–13, 2012.
- Dolbow, J.E. "Imposing Constraints Over Embedded Interfaces for Explicit Dynamics Calculations," The 17th International Conference on Finite Elements in Flow Problems, San Diego, CA, February 24–27, 2013.

5.2 Consultative and Advisory functions to other laboratories

John Dolbow serves as a consultant to Sandia National Laboratories, a DOE laboratory administered by Lockheed Martin. The focus of this consulting was the development of embedded finite element methods for fragmentation problems.

6 New Discoveries, Inventions, or Patent Disclosures

None to report at this time.

7 Honors / Awards

John Dolbow was named Yoh Family Endowed Chair at Duke University in 2009. He was also named co-editor of the archival journal *Finite Elements in Analysis and Design* in 2010.